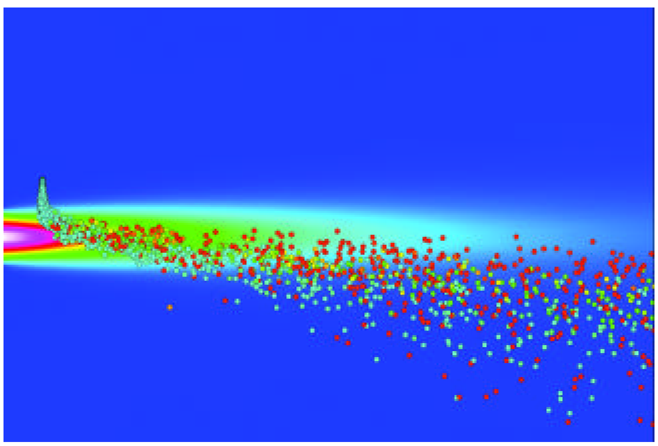
KEYWORDS ● Software ● Supercomputing ● Test & Measurement

Modeling and Simulation: Recreating the Real World

Modeling and simulation techniques have taken over many aspects of the R&D environment. From modeling the very labs that we work in to simulating the multiphysical world we live in.



Thermal spray process is visualized with Amtec's Tecplot. Color contours depict the axial plasma jet velocity while particle colors indicate the melt fraction (red is fully melted). The simulation was performed at the Idaho National Engineering and Environmental Lab.

It's human nature to simplify the physical world, to break apart complex physical phenomena into simpler more understandable terms, and then break it down into even simpler discrete components. Modeling and simulation are primarily mathematical representations of the real thing. A model is defined as a representation of a system that has been artificially created to better understand the real system. A simulation is then defined as a model operating in a discrete or continuous manner so that an observer can precisely determine the interactions between systems and components.

Computer-based modeling and simulation techniques have been available to researchers for several decades, becoming more sophisticated, more powerful, and more comprehensive every year. Most of the algorithms used in science- and engineering-based modeling and simulation techniques are based on traditional functional relationships. Continuing refinements to these algorithms, however, are made every year to make them more efficient and with higher resolution and accuracies. Computer hardware improvements have also made the processing of modeling and simulation techniques, many of which use computer-intensive iterative processes, more efficient and much faster. The power of the hardware not only allows researchers to obtain faster results, it also allows them to build larger, more intricate models that can then be solved in relatively workable timeframes.

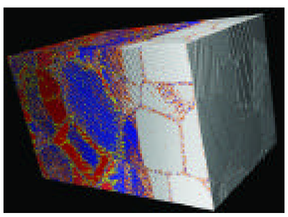
At the top end of this scale is the current reigning champion of supercomputers—the Earth Simulator (ES). Located in the Earth Simulator Center in Yokohama, Japan, this remarkable machine contains 5,120 NEC microprocessors, a relatively small number of processors as parallel supercomputers go, but operating with a peak performance of 40.96 Tflops (floating point operations/sec) and a sustained performance of 35.86 Tflops. This is about four times the performance of the second largest supercomputer now operating, the ASCI Q at Los Alamos (N.M.) National Laboratory (LANL)—one of two duplicate systems operating at the lab. Each ASCI Q (QA and QB) has a peak performance of 10.24 Tflops.

A 26.58 Tflops sustained performance was recently obtained on a spectral atmospheric general circulation model called AFES (AGCM for Earth Simulator). This simulation won the Gordon Bell Award at last November's IEEE SC2002 (Supercomputing 2002) conference in Baltimore, Md. The prestigious award recognizes the best performance in a practical application of parallel processors. The AFES simulation utilized the full 640-node (8 microprocessors/node) configuration of the Earth Simulator. These high-resolution global climate modeling capabilities allow scientists to study changes in the minute structures of the Baiu front (the rainy season seen in most parts of Japan) that are supposedly caused by the effects of global warming.

The AFES model produced climate details, such as tropical cyclones, never before seen with such reality on other modeling systems. The ES operators hope to conduct a few years of AFES climate simulations with 10-km or better grid resolution after only a few months of processing time on the ES. The continued improvement in supercomputers like the ES will improve both the resolution and the accuracy of climate models. About a third of the ES's operating time is dedicated to ocean and atmosphere modeling, the remainder is dedicated to solid earth modeling, computer science, and "epoch-making simulations"—those problems termed in the US scientific community as Grand Challenges.

From global to grain interface models

Researchers at LANL also use their supercomputing systems to simulate the dynamic deformation of materials. The primary purpose of these modeling systems is to address the safety, delivery, and performance issues for the aging US nuclear stockpile. Efforts to develop these advanced models involve many divisions within LANL and other US Dept. of Energy national labs, along with industrial and academic collaborators. Among the plethora of phenomena that the LANL researchers are modeling are material phase transitions and crystal reorientation at high rates of deformation. Theoretical investigations of length scales from nanometers (atomistic) to meters (structural) coupled with experiments are being pursued.



Molecular dynamics simulation performed at Los Alamos National Lab shows the propagation of a shock wave through a nanocrystalline material.

"Modeling of fluids and solid mechanics is one of the hottest modeling trends we currently study," says Frank Addessio, a project leader in LANL's Advanced Simulation and Computing (ASCI) program. The LANL Q system is currently the second largest supercomputer in the world with a peak performance of 10.24 Tflops. When completed, each Q

Disaster Modeling to Prevent a Reoccurrence

One of the most modeled and simulated physical systems ever developed was and is NASA's space shuttle orbiter. The Shuttle Columbia, being the first, heaviest, and oldest operational orbiter, was modeled extensively for everything including component and system design and development, launch dynamics, orbital docking, and landing and reentry dynamics. Obviously, with the loss of the Columbia on February 1, these computer simulations are being run nearly around the clock to come up with some scenario that could point to a cause for the reentry accident.

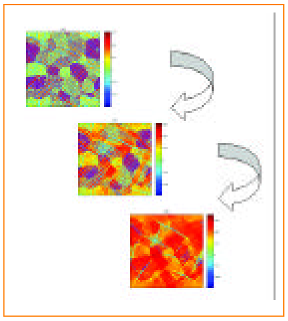
Two NASA Langley Research Center, Hampton, Va., Mach 6 wind tunnels have been reconfigured in this effort to investigate the thermal and environmental factors surrounding the reentry accident. The results from the wind tunnel tests will be combined with data from computational fluid dynamics (CFD) computer models. Langley researchers have performed numerous Mach 6 wind tunnel heating effects on the shuttle wings in previous design studies prior to the accident. NASA Ames Research Center, Moffett Field, Calif., also has a number of wind tunnels that could be put to some use. Ames also at one time had a supercomputer-based virtual wind tunnel

NASA researchers and investigators also, on occasion, take advantage of the wind tunnel capabilities at the US Air Force's Arnold Engineering Development Center in Tennessee.

Most NASA research centers had participated in the previous modeling studies on some part of the shuttle, making use of the various physical and theoretical simulation capabilities that exist across the NASA landscape. NASA Ames, for example, has a Flight Simulation Lab within which resides a vertical motion simulator, a computer-generated image lab, a virtual lab, and a cockpit graphics display lab, all of which have shuttle configurations and on-going experiments.

NASA's Advanced Supercomputing (NAS) Division at NASA Ames combines the data from experimental model studies in wind tunnels and other areas with high-end supercomputing capabilities. NASA Ames' high-end supercomputer is a 1,024 processor SGI Origin 3800 system that began operation last year.

One of the primary software tools being used in the Columbia investigation is likely the Cart3D, a high-fidelity inviscid analysis package for conceptual aerodynamic design. This computational fluid dynamics (CFD) software developed by Michael Aftosmis and John Melton at NASA Ames, in collaboration with Marsha Berger of the Courant Institute in New York was awarded NASA's software of the year in 2002.



Simulation of stressed polycrystalline iron-palladium was performed at Los Alamos National Lab. As twinned martensitic material at top is stressed preferred variants are favored, with the bottom final state having only the most favored (red) variants survive.

system (A, B, and C) will be combined with the others for a combined peak performance of more than 30 Tflops.

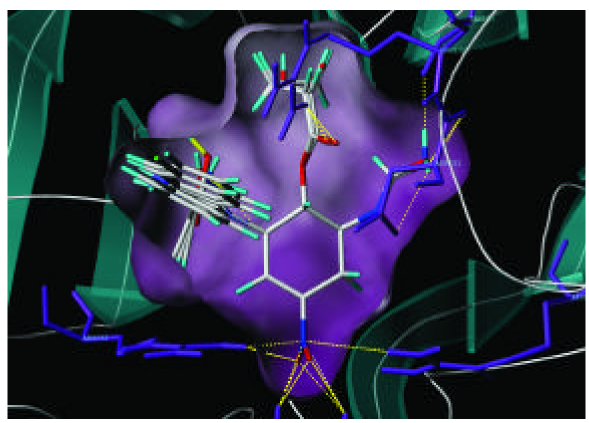
Plutonium-gallium metal alloys are relevant to the design of nuclear weapons and can be found in six different phase configurations that Addressio's research team studies. As temperature and pressure loads are applied to this material and it deforms beyond its elastic limit, it experiences a permanent deformation. These deformations result from the motion of defects or dislocations generally along the grain interfaces of the alloy. As a result of these and other deformation characteristics, it is important for LANL researchers to understand the specific elasticity, phase transformations, crystal reorientation, plasticity, and failure at the atomistic and granular characteristics of the material.

To study these materials at the different points in their operating environment, Addressio uses a number of traditional computational techniques to study their responses. At the smallest scale, molecular dynamics (MD) simulations are used to investigate the temperature and pressure induced phase transitions. Other techniques, such as Ginzburg-Landau (GL) theory are used to model the free energy of transforming crystal structures. Response characteristics of a large collection of crystals subjected to large deformations make use of homogenization techniques to determine the polycrystalline response. At larger scales (up to 1 m) macro-mechanical models are implemented with finite element and finite difference computer codes.

"Solid-state physics simulations currently look at the characteristics of about 10,000 atoms with models running on supercomputers, like our ASCI Q machines," says Addessio. "Molecular dynamics models and simulations look at up to a million atoms." Development of code and computer systems that can bridge the gaps between the solid-state systems and macromolecular structures with better physics models will provide the researchers with better overall answers, he says. These systems do not yet exist, but it is a current area of intense R&D.

While the algorithms for these simulations continue to improve ("...and have improved substantially over the past several years," says Addessio), there are a number of areas, such as automated mesh generation, that require continued improvements. "If you're doing a Lagrangian deformation, you may have to generate a new mesh after several iterations," says Addessio. The imprecise nature of nonlinear solvers also needs continued enhancements, he says.

Another modeling application of LANL's supercomputers is to simulate the biological processes that remove existing - bone and deposit new bone in human physiology models. Removal and regrowth of bone occurs normally in humans during growth periods, repair of injuries, in response to physicochemical factors such as stress or exercise, and during hormonal changes. Researchers, led by Nicholas Metropolis, utilize well-known and understood Monte Carlo techniques to analyze these bone changes. Monte Carlo modeling techniques are well-suited to the multistate, nonlinear biological systems.



X-ray structure of influenza virus neuraminidase with five ligands that are predicted to be active was generated with Tripos' RACHEL software. Hydrogen bonds between the ligands and residue are indicated by dashed yellow lines. Dark purple regions contain a greater acceptor/donor density and light purple regions indicate areas where hydrogen bonding is less likely to occur.

These models are also used to study age-induced osteoporosis, manned space flight induced low-g bone loss that is partially non-reversible, and the correlation of bone structure to its mechanical properties.

A relatively new large modeling and simulation program surrounds the National Fusion Collaboratory (NFC). This on-going three-year project represents a fundamental paradigm shift for the fusion research community where data, analysis and simulation codes, and visualization tools are created and used as network tools. The program will eventually consist of more than a thousand researchers from more than 40 institutions, including the US Dept. of Energy's Argonne and Lawrence Berkeley National Labs, the Princeton Plasma Physics Lab, SCI Institute, General Atomics, and others. The network will require significant investments in computer science research to extend the existing toolkits available beyond their present capabilities. A Globus-enabled implementation of the NFC's MDSplus data repository framework was demonstrated at SC2002 this past November. Globus is an open architecture, open source software toolkit that enables researchers to develop useful computer network, or grid, applications and programming tools. Globus was a 2002 R&D 100 Award winner developed by Ian Foster's research group at Argonne National Lab.

Visualizing data

Modeling and simulation systems generally rely on simplified visualizations to display their results. Here, too, the problems encountered in going from micro- to macro-scale models create issues in the basic visualization tools used by researchers. Modeling a telephone cable running across a windy valley, for example, is a complex problem because of the boundary layers around the cable. Modeling the cable by itself can be achieved relatively easily with a simple grid system containing only a few hundred nodes. Creating the computational grid around the entire cable that takes into effect its surrounding environment could require as many as a million to one increase in the number of nodes.

"We've been able to solve the preprocessing problems involved with building complex models," says Mike Peery, president of Amtec, Bellevue, Wash. "But, building the grids that define the space is still the biggest problem in modeling." Amtec's Tecplot visualization tool is used by researchers to visualize large sets of modeling data. Tecplot can load and plot modeling data organized in a variety of grid structures used in computer programs to simulate specific physics characteristics, such as fluid dynamics, electromagnetics, and heat transfer. The data points in Tecplot can be arranged in multiple blocks of rectangular and body-fitted curvilinear grids, unstructured finite element grids made of triangles, quadrilaterals, prisms, and bricks. It can also interpolate random and irregular data into grid structures and even triangulate the data points.

Specialized tools

A number of analysis and visualization tools are available to researchers for building, developing, and analyzing models and simulations. Fluent, Lebanon, N.H., and CFDRC, Huntsville, Ala., supply computational fluid dynamics (CFD) tools for modeling liquid and gaseous flows around objects. MSC.Software, Santa Ana, Calif., has a number of specialized software systems for simulating specific physical systems in a model. These include acoustical response, finite element stress modeling, thermal analysis, dynamic response systems, fatigue, flight loads, noise, vibration, harshness, and nonlinear responses.

Algor, Pittsburgh, Pa., also specializes in a number of different areas. They have products that focus on mechanical event simulations, multiphysics, heat transfer, FEA, CFD, MEMS analyses, electro-statics, civil engineering, and NASTRAN computer-aided engineering.

Noran Engineering, Los Alamitos, Calif., also is a supplier of NASTRAN tools. NASTRAN was originally developed by NASA researchers as a structure-based finite element analysis tool. NASA's structural analysis system, or NASTRAN, was targeted at solving large problems that

Colorful Computers

The Advanced Simulation and Computing (ASCI) program is a collaboration between the US Dept. of Energy's Sandia, Livermore, and Los Alamos National Laboratories to support and monitor the US nuclear stockpile. Each of these labs has large supercomputing facilities to support this research. The largest of these is the IBM-supplied 100 Tflops ASCI Purple (following the ASCI White and Blue-Pacific systems already installed), which will be installed at Livermore in late 2004. Purple, a fifth generation ASCI supercomputer, will contain more than 12,000 IBM Power5 microprocessors and nearly 50 TB of memory.

IBM is also supplying a BlueGeneL supercomputer to Livermore, which is modeled after its own BlueGene system being used to model DNA folding in its Life Science division.

used the best available algorithms for solving matrix equations and eigenvalue analyses. To continue development of the code as a commercial product, NASTRAN's source code was made available to software companies by NASA.

Life science modeling

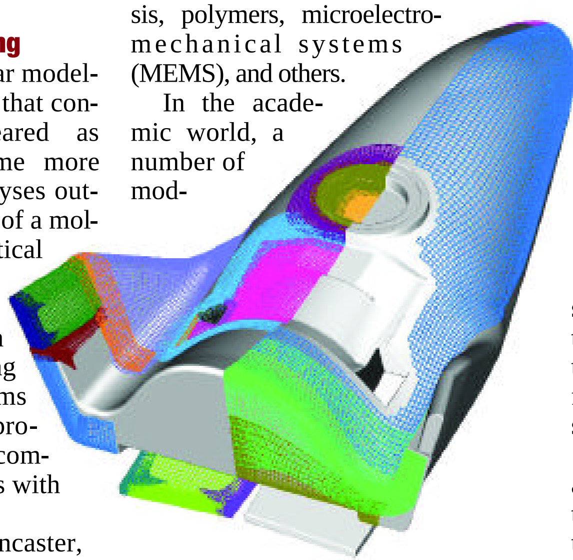
It used to be called molecular modeling about 10 years ago. But that connotation quickly disappeared as software developers became more focused on specialized analyses outside of just the visualization of a molecule. Today, pharmaceutical and biotech companies rely heavily on a number of modeling and simulation tools for modeling everything from entire biological systems to simulating genomic and proteomic drug discovery compounds and their interactions with cells and diseases.

Simulations Plus in Lancaster, Calif., for example, has a product called GastroPlus that simulates the absorption and pharmacokinetics for orally dosed drugs. The underlying model for GastroPlus is the advanced compartmental absorption and transit model. GastroPlus is used to perform automated analyses, such as virtual clinical trials. The software also can compare how a drug dose dissolves in the laboratory to how it behaves in humans and animals. Other products from Simulations Plus can estimate a number of ADME (absorption, dissolution, metabolism, and excretion) properties of new chemical entities (NCEs) from their molecular structure.

After a series of M&A's over the past 10 years, San Diego-based Accelrys and St. Louis-based Tripos are the two remaining largest life science modeling and simulation companies. Both offer a full range of molecular design and analysis tools. SYBYL is Tripos' foundation product for drug discovery, providing the fundamental components for understanding molecular structure and properties with a special focus on the creation of NCEs. SYBYL has the essential construction, editing, and visualization tools for both large and small molecules.

In addition to its life science simulation tools, Accelrys also has a number of tools and collaborations in non-life science molecular modeling, such as in solid state chemistry, catalysis, polymers, microelectromechanical systems (MEMS), and others.

In the academic world, a number of modeling tools are available, including software tools like Coposer, Congen, CPH Models, Dragon, ICM, Insight, Modeller, Quanta, and Seiss-Mod, among others. Similarly, visualization tools like CHIMERA, SWISS-PDB-Viewer, RasMol, and Pymol are available.



Creating finite element and finite difference grids that support the appropriate stressed areas in a product like NASA's X38 Crew Return Vehicle is the first step in running various simulation studies. NASA's Advanced Supercomputing Division at their Ames Research Center has created an Information Power Grid (IPG) Virtual Lab that automates and monitors various simulated parametric studies.

Other tools too numerous to mention

While this discussion focused on the most popular physical and biological modeling and simulation tools currently being used by researchers, there are a number of other peripheral tools that continue to draw interest from niche groups. Fully immersive modeling systems continue to evolve, albeit slowly. Virtual reality CAVE environments and video-enabled virtual modeling systems have found a few strong applications, but are limited in further expansion due to cumbersome software and limited real value.

Combining the modeling capabilities of several software programs into an integrated system is also done, although rarely due to the incompatibility of most interfaces. Modeling and simulation studies in the planning of attacks on Iraqi chemical and biological warfare targets, for example, have been done for more than three years. While these systems are less mature than conventional warfare modeling capabilities, the fact that they have been performed for several years gives them some serious recognition values.

Virtual modeling has found strong applications in military areas as virtual training and simulation based solutions to minimizing the risk of losing human lives. Virtual tank training, virtual flight training, and virtual bioterrorism events have become real-life video game extensions with proven value in both cost and speed to achieving certain levels of capabilities.

—Tim Studt

>> Resources

Accelrys, 800-756-4674, www.accelrys.com
Algor, 800-482-5467, www.algor.com
Amtec Engineering, Inc., 800-763-7005, www.amtec.com
CFDRC, 256-726-4800, www.cfdrc.com
Earth Simulator, 81-45-778-5863, www.es.jamstec.go.jp
Fluent, Inc., 603-643-2600, www.fluent.com
Los Alamos National Laboratory, 505-667-7000, www.lanl.gov
MSC.Software Corp., 714-540-8900, www.mscsoftware.com
NASA Advanced Supercomputing Division (NASA Ames Research Center), 650-604-4502, www.nas.nasa.gov
NASA Langley Research Center, 757-864-1000, www.larc.nasa.gov
National Fusion Collaboratory, www.fusiongrid.org
Noran Engineering, 877-636-2787, www.NENastran.com
Simulations Plus, Inc., 661-723-7723, www.simulations-plus.com
Tripos, 800-323-2960, www.tripos.com